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Formulating LUTI Calibration As an Optimisation Problem: Estimation of Tranus Shadow Price and Substitution Parameters

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Abstract

Cities and their employment catchment areas are focus points of economic activity, transportation, and social interactions. The need for land use and transport **integrated** modelling (LUTI modelling) as a decision aid tool in urban planning, has become apparent. Many LUTI models have been developed starting in the 1960's and especially in the last 15 years. Instantiating such models on cities, requires a substantial data collection, model structuring and parameter estimation effort; for conciseness, the latter is referred to here as **calibration**. This work is a partial effort towards the integrated calibration of LUTI models. It considers one of the most widely used LUTI models and softwares, Tranus. The usual calibration approach for Tranus is briefly reviewed. It is then reformulated as an optimisation problem, in order to make it amenable to the systematic incorporation of constraints on parameters and additional data and to form a clear basis for future fully integrated calibration. The problem at hand concerns a dynamic system; an approach is shown how to "eliminate" parts of the dynamics in order to ease the parameter optimisation. We also discuss how to validate calibration results and propose to use synthetic data generated from real world problems in order to assess convergence properties and accuracy of calibration methods.

Introduction

Transportation and land use planning were traditionally carried out in a decoupled manner: although land use is naturally a main input for transportation planning, the impact of changes in transportation infrastructure or policies, on land use, was often ignored. One typical such impact is urban sprawl, whose causes include the dynamic feedbacks between transportation and land use. Neglecting such feedbacks in modelling systems that assist decision making, may lead to incorrect assessments of transportation plans for instance.

For this reason, the need for land use and transport **integrated** modelling (LUTI modelling) as a decision aid tool in urban planning, has become apparent. Many LUTI models have been developed starting in the 1960's (Wegener 2004) and especially in the last 15 years. Instantiating such models on cities or regions, requires a substantial data collection, model structuring and parameter

estimation effort; for conciseness, the latter is referred to here as **calibration**, knowing that model structuring (definition of the appropriate granularity of spatial zones, socio-economic groups and activities, and the representation of the transportation network) is often also considered to be an integral part of model calibration. Calibration of large-scale LUTI models is a challenging task, due to their non-linear and dynamic nature and the potentially large number of parameters. It is usually partitioned into a set of smaller, partial parameter estimation problems of individual components of a model, and an integrated calibration of the composite model, taking into account the mutual interactions between these components, is most often lacking (a notable exception is the set of calibration approaches developed for the MEPLAN model, see (Abraham 2000; Abraham and Hunt 2000)).

This work is a partial effort towards the integrated calibration of LUTI models. It considers one of the most widely used LUTI models and softwares, Tranus (de la Barra 1999). In the following, we first briefly review this model and its usual calibration approach. We then reformulate its calibration as an optimisation problem, in order to make it amenable to the systematic incorporation of constraints on parameters and additional data and to form a clear basis for future fully integrated calibration. We first show a solution of the optimisation problem for a subset of model parameters before describing a means of automatically estimating two parameter sets that usually were considered partly interactively. The problem at hand concerns a dynamic system; an approach is shown how to "eliminate" parts of the dynamics in order to ease the parameter optimisation. Finally, we discuss how to validate calibration results and propose to use synthetic data generated from real world problems in order to assess convergence properties and accuracy of calibration methods, a proposal that seems to be novel for LUTI models.

Overview of the Tranus LUTI Model and its Usual Calibration Approach

Tranus (de la Barra 1999) provides a generic framework for modelling land use and transportation in an integrated manner, at urban, regional, or national scales. The region of interest is divided into *spatial zones* and *economic sec-*

tors. Then Tranus combines two main modules: the *land use and activity* module which simulates a spatial economic system by modelling the locations of activities and the interactions between economic sectors, and a *transportation* module, which dispatches transportation demands arising from economic activities to a model of the transport network. These two modules interact: first, as mentioned, transportation demand is generated by economic activities (including for instance home-to-work trips, but also trips to schools, for shopping, freight etc.). Second, the generated mapping of trips to the transportation network, leads to modified costs and disutilities of traveling (e.g. congestions, travel times), which are fed back to the land use and activity module where they impact the location of businesses and households and the “economic market” (the total price of goods for instance depends on transportation costs). Figure 1 represents these interactions. The two modules use discrete choice logit models (McFadden and Train 2000), linked together in a consistent way. This includes activity-location, land-choice, and multi-modal path choice and trip assignment.

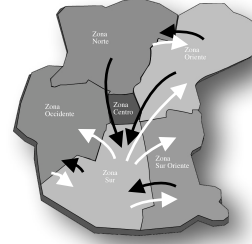
Tranus is a macroeconomic equilibrium type model: the above two modules are run iteratively until an equilibrium is reached, as illustrated by figure 1. To be precise, three instances of equilibria are considered. First, the land use and activity module aims at achieving an economic equilibrium between offer, demand and prices, given current transportation costs and disutilities. This is further explained below. Second, the transportation module generates an equilibrated (or, optimal, in a specific sense) mapping of transportation demand to the network. Finally, the modules are run iteratively until a global equilibrium is reached, i.e. where neither land use nor transportation use, evolve anymore.

We now describe the land use and activity module, whose calibration this paper addresses, in more detail. Three main types of economic sectors are usually modelled: floorspace or land sectors (usually, at least two or three types of residential floorspace, such as detached houses, apartments, social housing, etc.), households (usually, one models several socio-economic groups, based on income and/or household composition for instance), and businesses. The latter comprise industries (whose main output is dedicated to exportation) and services (schools, hospitals, leisure, commercial services, etc.). Following economic base theory (see for instance (Lowry 1964)), export-oriented industry generates demands of households (workers) and service businesses. The latter in turn generate demand on further households. Vice-versa, households also consume services. Finally, all businesses and households consume floorspace (or land).

Floorspace is located in the modelled spatial zones. Thus, the “consumption” of households by businesses for instance, will generate a demand for transportation between zones (home-to-work trips). All mentioned economic activities are represented by productions and demands, resulting in prices. The equilibrium between these depends further on various economic parameters that aim at representing the behaviour of people and businesses, such as demand elasticities and variables representing the general attractiveness of zones (beyond land rent). **Productions** X_i^n express how

LAND-USE

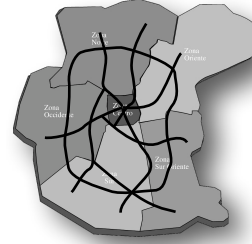
Simulate the location of activities in space, land use, the real estate market.



X_i^n Production of the activity of type n in the zone i
 p_i^n Price of consuming the activity of type n in the zone i

EQUILIBRIUM

TRANSPORT



f_{ij}^n Transported flux of activity type n from zone i to zone j
 t_{ij}^n Cost of transporting the activity type n from zone i to zone j

Computes the transportation demand, and affects it to available transport resources.

Figure 1: Schematic overview of Tranus.

many “items” of each economic sector n are present in each zone i . **Demands** D_i^{mn} express how many items of a sector n are demanded by the part of sector m located in zone i . Finally, p_i^n defines the **price** of (one item of) sector n located in zone i . Here, “price” is dictated by land or floorspace prices, which are true prices, whereas the “price” of a household (roughly speaking, its demand for salary) is derived from the floorspace occupied by the household.

All these variables are computed from one another by a system of about a dozen equations, see (de la Barra 1999) for details. Since they depend on one another (for instance demand generates production and vice-versa), we are in the presence of a dynamic system. A sketch of the central parts of this system is shown in figure 2, where we omit many details in order to make this paper as self-contained as possible. It shows the sequence of computations done in Tranus’ land use module. At each iteration of the process, current prices are fed into the computation of demand (via intermediate variables not detailed here) which in turn are fed into the computation of production. Given the new distribution of production across sectors and zones, production and consumption costs are computed (marked as c in the figure), based on the current prices and transportation costs. These are then used in the next iteration to determine new prices, and the above computations are repeated. The entire process starts from floorspace/land prices, which are given via collected data and production destined for exportation outside the area of study, which is also given. It is repeated until convergence; concretely, until convergence of productions X and prices p (this implies convergence of all other variables).

The subset of model equations relevant to this paper, is as follows. Demand is computed for all combinations of zone i , demanding (consuming) sector m and demanded sector n :

$$D_i^{mn} = (X_i^{*m} + X_i^m) a_i^{mn} S_i^{mn} \quad (1)$$

$$D_i^n = D_i^{*n} + \sum_m D_i^{mn} \quad (2)$$

where X_i^{*m} is the given exogenous production (for exports), X_i^m the induced endogenous production obtained in the previous iteration (or initial values), and D_i^{*n} exogenous demand. D_i^n in (2) then gives the total demand for sector n in zone i . a_i^{mn} is a technical demand coefficient and S_i^{mn} is the substitution proportion of sector n when consumed by sector m on zone i (explained later in more detail).

In parallel to demand, one computes the **utility** of all pairs of production and consumption zones, j and i :

$$U_{ij}^n = p_j^n + h_j^n + t_{ij}^n. \quad (3)$$

Here, t_{ij}^n represents transport disutility. Since utilities and disutilities are difficult to model mathematically (they include subjective factors such as the value of time spent in transportation), Tranus incorporates adjustment parameters h_j^n , so-called shadow prices, amongst the model parameters to be estimated.

From utility, we compute the probability that the production of sector n demanded in zone i , is located in zone j . Every combination of n , i and j is computed:

$$Pr_{ij}^n = \frac{A_j^n \exp(-\beta^n U_{ij}^n)}{\sum_h A_h^n \exp(-\beta^n U_{ih}^n)}. \quad (4)$$

Here, h ranges over all zones, A_j^n represents attractiveness of zone j for sector n and β^n is the dispersion parameter for the multinomial logic model expressed by the above equation.

From these probabilities, new productions are then computed for every combination of sector n , production zone j and consumption zone i :

$$X_{ij}^n = D_i^n Pr_{ij}^n. \quad (5)$$

Total production of sector n in zone j , is then:

$$X_j^n = \sum_i X_{ij}^n. \quad (6)$$

Given the computed demand and production, consumption costs are computed as

$$\tilde{c}_i^n = \frac{\sum_j X_{ij}^n (p_j^n + tm_{ij}^n)}{D_i^n} \quad (7)$$

where tm_{ij}^n is the monetary cost of transporting one item of sector n from zone j to zone i .

These finally determine the new prices:

$$p_i^m = VA_i^m + \sum_n a_i^{mn} S_i^{mn} \tilde{c}_i^n \quad (8)$$

where VA_i^m is value added by the production of an item of sector m in zone i , to the sum of values of the input items.

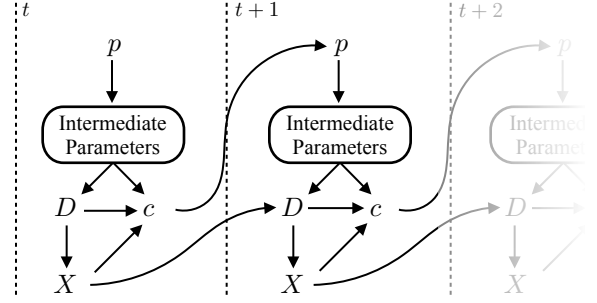


Figure 2: Sketch of computations in the land use and activity module.

Calibration. A model like Tranus is a simplification of reality, that enables to get insights on the economical activity of a city. The calibration process consists in adjusting the model such as to reproduce the actual observed behaviour of a study area in a given timeframe or base year. It is usually performed by experts and is based on a mix of numerical parameter estimation procedures, interactive trial-and-error, and assessment of the model calibration against observed data and expert opinion. Once a LUTI model's parameters are calibrated using data from a base year (or possibly multiple base years), the usual application of a model is to use it to predict the evolution of land use and transportation usage, for different alternative scenarios of future changes in development strategies, transportation infrastructure, fiscal policies, etc.

The calibration of the land use module is usually done by a hierarchical process of the following type. The model parameters are split in three sets: (i) parameters that are computed independently from all others using appropriate data, (ii) the shadow prices h_j^n (adjustment parameters) of equation (3), (iii) and all remaining parameters. The latter two sets of parameters are estimated in an iterative process: given initial values of the third set of parameters, one estimates shadow prices for which the model, after convergence, reproduces the productions X_0 observed in the study area. Then, the remaining parameters are updated using additional observations and constraints on the shadow prices: one wants to make these as small as possible. This process is repeated interactively by the expert modeller until a compromise deemed satisfactory, is achieved between model fit, constraints, and plausibility of the estimated economic parameters.

As for the estimation of the shadow prices, a simple method is used: at the end of each iteration (cf. figure 2 and the above equations), shadow prices are updated as follows:

$$h_i^{n,t+1} = (h_i^{n,t} + p_i^{n,t}) \frac{X_i^{n,t}}{X_{0,i}^n} - p_i^{n,t+1} \quad (9)$$

The rationale is to increase shadow prices if the production computed by the model exceeds observed production and vice-versa, so that in the next iteration, computed productions hopefully come closer to observed ones. So computation of shadow prices in iteration $t + 1$, depends on the

values of the productions and prices at iteration t , as shown in equation (9).

Proposed Calibration Approaches

Our main motivations are to replace the sequential calibration process outlined above by a process that rigorously estimates as many parameters as possible, taking into account all available constraints and assumptions in a systematic manner, to automatise as much as possible the calibration process, and to make it more reproducible. We believe that a natural way of achieving these goals is to explicitly formulate the calibration process in terms of a cost function (or possibly, as a multi-criteria decision problem) that is to be minimised or maximised, with respect to a set of constraints, when given. This is for example not directly the case in the existing approach, where the estimation of shadow prices and other parameters is done without a definition of a clearly defined cost function. Formulating calibration via explicit cost functions enables to use the rich variety of optimisation algorithms existing in the literature and in numerical libraries.

A first step in this direction concerns the estimation of shadow prices, a second step deals with the automatic estimation of both shadow prices and other parameters; these two steps are described in the following.

Optimisation of Shadow Prices

As explained above, the goal is to estimate shadow prices for which productions computed by the model are equal or as similar as possible, to observed productions. This can be directly cast as a minimisation problem:

$$\min_h \|X(h) - X_0\|^2. \quad (10)$$

Here, h is a vector containing all shadow prices, X_0 the vector of observed productions, and $X(h)$ the vector of productions computed by the model, after convergence of the iterative process shown in figure 2. The dependency of these on the shadow prices is visible from equations (3) to (6).

One problem is that productions $X(h)$ are only available after convergence of our dynamic system of equations. Consequently, the computation of the gradient of the cost function (be it analytical or by numerical approximation) or any other variables needed by a chosen optimisation method, may be complicated or requiring waiting for convergence too. In order to solve this problem, we observe that one may cut through a loop in our dynamic system and directly compute demand and production that are in equilibrium: in the iterative scheme shown in figure 2, the computation of demand and production only involves equations that are linear in these parameters, cf. (1), (2), (5), and (6). These equations may be re-organised in order to form a single linear equation system in the productions and demands. However, since only productions are needed in the cost function, one may reduce the problem to only estimating these (demands may be computed from estimated productions by substitution if required). To do so, we substitute D_i^n in equation (5)

using equations (1) and (2), giving:

$$X_{ij}^n = \left\{ D_i^{*n} + \sum_m (X_i^{*m} + X_i^m) a_i^{mn} S_i^{mn} \right\} Pr_{ij}^n \quad (11)$$

Upon substituting this into (6), we obtain:

$$X_j^n = \sum_i \left\{ D_i^{*n} + \sum_m X_i^{*m} a_i^{mn} S_i^{mn} \right\} Pr_{ij}^n + \sum_i \sum_m a_i^{mn} S_i^{mn} Pr_{ij}^n X_i^m. \quad (12)$$

These equations, for all sectors n and zones j , form a single linear equation system in the productions X_j^n . Note that by construction, solving this system and inserting the resulting productions in the equations defining demand, will lead to demands that are in equilibrium with the productions.

Still, two further problems remain. First, it seems difficult to compute the gradient of the cost function (10) analytically. Numerical differentiation using finite differences is possible but would be expensive (every finite difference would require the solution of a linear equation system of type (12)). Second, although productions and demands computed as above are in equilibrium, the prices p may still evolve from the current to the next iteration. Hence, one still has to iterate model equations until prices converge.

Our solution to the first remaining problem is to exploit the fact that we do have observed productions: we simply substitute these into the right-hand side of (12), which allows to directly compute modelled productions as opposed to having to solve a large linear equation system.

As for the second problem, we add the prices to the set of parameters to be optimised: with reference to figure 2, we use current estimates of price parameters as input to each iteration and then compare how close they are to the prices computed at the end of each iteration. In terms of equations, price parameters are inserted in equations (3) to (7) and then compared to the results of prices computed by the model via (8). The discrepancy between these is added as a new term to the cost function (10), leading to our final optimisation problem:

$$\min_{h,p} \|X(h, p, X_0) - X_0\|^2 + \|\hat{p}(h, p, X_0) - p\|^2 \quad (13)$$

Here, \hat{p} is the vector of prices computed by the model using (8) and the notation $X(h, p, X_0)$ shows that modelled productions are computed as explained above by substituting observed productions X_0 into the right-hand side (12).

Note that all terms in the above cost function, as well as their partial derivatives, can be computed in closed-form as functions of the unknowns h and p . This enables efficient computations of the ingredients of any least squares or other optimisation method; in our implementation, we use the Levenberg-Marquardt method (Levenberg 1944) to solve problem (13).

Let us also note that other choices than the L_2 norm would of course be possible to define the cost function of (13). We may also weight the two terms differently, in order to favour equilibrium in production over that in prices or vice-versa in cases where a global equilibrium cannot be reached.

Optimisation of Shadow Prices and Substitution Parameters

Tranus models include a discrete choice sub-model that represents the households' ability to choose among different types of residential buildings (i.e., floor space). That choice is captured in the "substitution model". The functionality of substitution models is rather broad, encompassing goods and services other than floor space and agents other than households. In practice, substitution models typically apply to households' consumption of land for residential purposes, businesses' consumption of floor space for offices and factories, and construction companies' consumption of land for building sites. Substitution models are challenging to calibrate for several reasons, including the large number of parameters. Two additional reasons are salient. Because the range of plausible values is large, selection of the parameters' initial values is typically made with little confidence. We propose a hybrid and multiphase process for calibrating substitution models. In the first phase, certain parameters' initial values are estimated with a multinomial logistic regression (Train 2009). In the subsequent phases, mathematical optimisation is used to fine-tune the estimated parameters and to calibrate the other substitution model parameters. With our proposed approach, the process of determining parameter values is fast, replicable, and entirely transparent. Another important benefit is that substitution models are less likely to be overfitted, which is a hazard with the current and universally used calibration practice that sets floor space and land "attractors" to the value of base production (see below).

Tranus's substitution model for stock sectors (floor space and land): the basics. For ease of exposition, the stock sectors will be referred to as "floor space" (sector n), and the consumers of floor space will be referred to as "households" (sector m). In Tranus's substitution model, the proportion of sector m households in zone i that consume floor space sector n , S_i^{mn} , is given by the well known logit formulation (McFadden and Train 2000):

$$S_i^{mn} = \frac{W_i^n \exp(-\omega^{mn} a_i^{mn} \tilde{c}_i^n)}{\sum_{p \in K^m} W_i^p \exp(-\omega^{mp} a_i^{mp} \tilde{c}_i^p)} .$$

Here, K^m represents the set of substitutes that sector m has access to, for example, for "rich" households m , this could be $K^m = \{\text{condos, detached houses}\}$. Using Tranus terminology, W_i^n is an "attractor", a parameter that represents attributes of floor space sector n other than cost (utility); it is specified (and potentially calibrated) for each zone in which sector n is present. It is common practice to set each attractor to the value of base production, i.e., $W_i^n = X_{0i}^n$, the production of floor space sector n observed in the base year. The term a_i^{mn} is the average sector m household's consumption of sector n floor space; \tilde{c}_i^n is the consumption cost of sector n floor space (per unit of floor space), see (7); ω^{mn} is the penalising factor, which is specific to both household sector m and floor space sector n ; and the product $a_i^{mn} \tilde{c}_i^n$ may be interpreted literally as a household's expenditure on housing (say, per month). After

S_i^{mn} has been calculated, it is used to determine the demand D_i^{mn} of the sector m households in zone i for floor space sector n , cf. equation (1). In that equation, X_i^{*m} represents the exogenous households and X_i^m represents the endogenous ones.

- Phase 1: estimating parameters' initial values with multinomial logistic regression.** The substitution model's parameters are estimated with multinomial logistic regression (Train 2009). The data that are essential for estimation are household level observations on floor space consumption, housing expenditure, and the Tranus sector to which the household belongs. The dependent variable in a regression will be the choice of floor space sector, and the independent variable is the housing expenditure. The regressions are conducted separately for each household sector, and they yield estimates of $-\omega^{mn}$ for each combination of floor space sector and household sector. To match Tranus's formulation of the unscaled utility, a constant cannot be included in the regressions¹. Assuming that the coefficients on expenditure have the expected negative sign, the absolute values of the coefficients are the penalising factors' initial values. Assuming that there are two household sectors ($n = 1, 2$) and three floor space sectors ($m = 11, 12, 13$), the regressions provides estimates of $-\omega^{1,11}$, $-\omega^{1,12}$, $-\omega^{1,13}$, $-\omega^{2,11}$, $-\omega^{2,12}$, and $-\omega^{2,13}$.
- Phase 2: fine tuning the penalising factors.** The penalising factors estimated in Phase 1 probably still need to be fine tuned to reduce the differences between the predicted production of floor space and the observed production of floor space. Fine tuning probably would also be necessary to achieve reasonable values of the floor space sectors' shadow prices. Computing the induced production X of the land use sectors is much easier than other type of sectors. This is mainly because the land use sectors don't depend on the Transportation module of Tranus. The other big advantage is that the prices are not endogenous, they are known and fix. This makes computing the the induced production straightforward for a given set of shadow prices of the land use sectors.

The cost function presented in equation (13), is reduced to:

$$f(h) = \|X(X_0, h) - X_0\|^2 .$$

Let us define \mathcal{L} as the set of land-use sectors. If we consider all of Tranus' parameters fixed except the parameters ω then we can rewrite the cost function as:

$$f((h^n)_{n \in \mathcal{L}}; \omega) = \sum_{n \in \mathcal{L}} |X^n - X_0^n|^2 .$$

In a perfectly fitted model, the shadow prices would be equal to zero. What we propose is find the ω values for $h^n = 0, \forall n \in \mathcal{L}$ that minimise the problem:

$$\min_{\omega \in \Omega} f(0, \omega) \quad (14)$$

¹If the attractors W_i^n are different from 1, the constant in the logistic regression could account for some of their value.

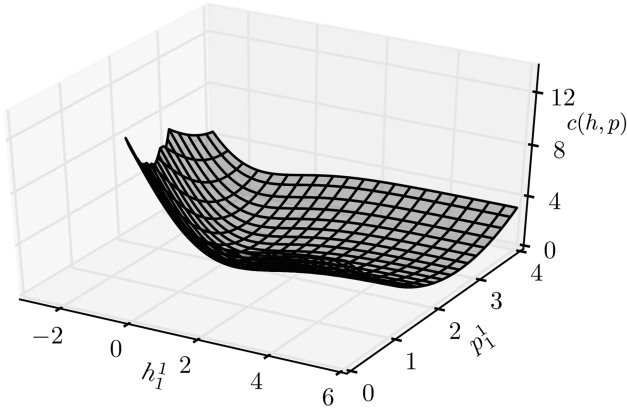


Figure 3: Plot of cost function for a given pair (h_1^1, p_1^1) near the optimal value $(0, 2.676)$.

where Ω is a set of bounds over the penalising factors ω . We used a conjugate-gradient algorithm to solve this problem, and the starting points are the values obtained from the Multinomial Logistic regression of Phase 1. If we call ω^* the solution of (14), then the final values for the shadow prices for the land use sectors are:

$$h^* = \arg \min_h f(h, w^*) .$$

Results

Generation of Synthetic Data with Ground Truth

Results of Shadow Price Calibration

We applied our approach to the *Example_C* model from the Tranus website, a small model with 3 zones and 5 sectors. First, we generated synthetic data from that model as described just above, with shadow prices $h_i^n = 0$ for each sector n and zone i . As expected, the cost function is zero at $h = 0$, and increases its value when we get away from the optimum. The cost function appears to be locally convex near the optimal value, cf. figure 3.

If we consider for example sector 1 and zone 1, we can plot a “slice” of the cost function (13) near the optimal value $h_1^1 = 0, p_1^1 = 2.676$ as shown in figure 3. Here we can observe that as the shadow price gets larger the cost increases up to a plateau state ($X_1^1(h) \rightarrow 0$). In the case of the price p , if we move away from the optimal value $p = 2.676$, the cost increases quadratically.

We tested the robustness of the optimisation scheme with 1,000 random initial sets of shadow price values; the optimisation procedure outlined in this paper always converged to the ground truth solution. The initial values of shadow prices in these random trials were generated from a uniform distribution in $[-10, 10]$, which is highly representative (prices are in the interval $[0, 4]$ and nearly all shadow prices of a model are in practice smaller than the corresponding prices).

Results of Estimation of Shadow Prices and Substitution Parameters

We applied this procedure to a real-scale LUTI model for North-Carolina, with 38 zones, 3 floorspace and 9 other eco-

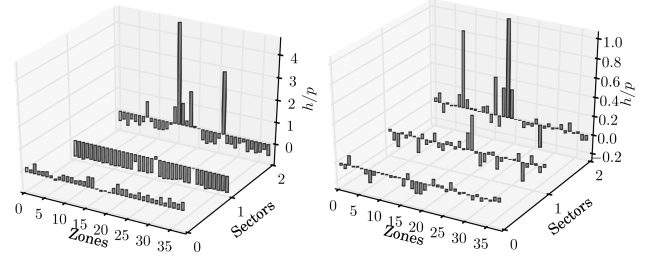


Figure 4: Ratios of shadow prices and prices after phase 1 (left) and 2 (right). Note the different scales of the graphs.

nomic sectors. Figure 4 shows the shadow prices for all zones and floorspace sectors, after the two phases of our process. After each phase, a global equilibrium of demand, production and prices, is achieved, however after the novel second phase, shadow prices are much smaller, meaning that the model represents reality much better (small ratios of shadow prices over prices is a crucial criterion used by practitioners to assess the quality of a Tranus LUTI model).

Conclusions and final remarks

We have developed an optimisation methodology that gives us a partial calibration of Tranus. Secondly, we have proposed a technical contribution to the way equilibrium equations of X and p are handled in Tranus, permitting us to decouple a double fix point optimisation problem. Additionally, the procedure of generating synthetic data files for testing the calibration methodology is a practical way to test and check the performance of a general calibration scheme. Finally, we have proposed a practical and efficient way of calibrating the substitution parameters, providing a methodology that produces significantly better than the usual approach, and in a shorter time due to its full automation.

Next steps will be the simultaneous optimisation of shadow prices and substitution parameters and eventually, of other model parameters, fully integrated and automatic calibration being our ultimate goal. **Acknowledgment:** This work is supported by the CITiES project (ANR-12-MONU-0020).

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